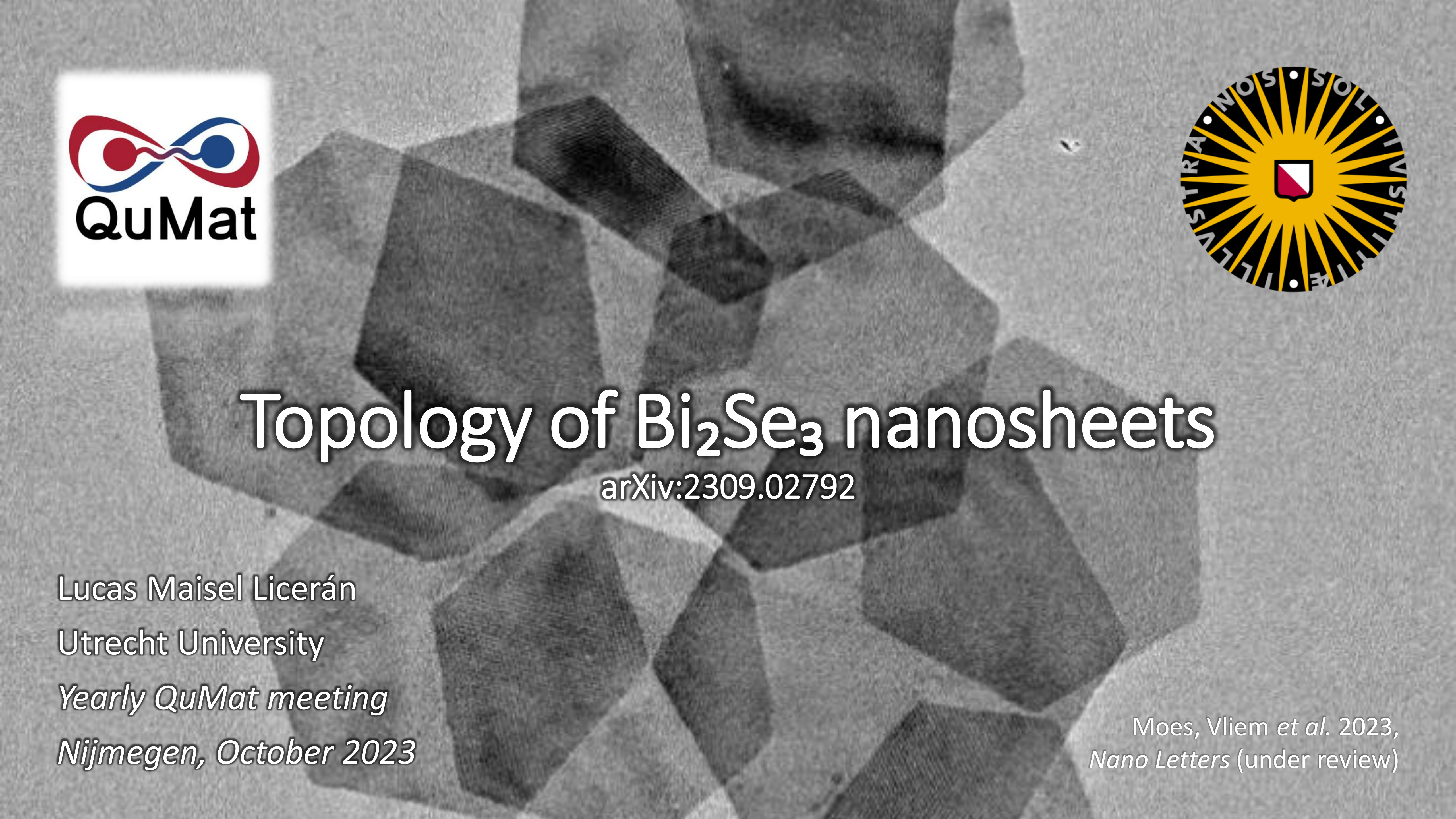

Topology of Bi_2Se_3 nanosheets

arXiv:2309.02792

Lucas Maisel Licerán
Utrecht University

Yearly QuMat meeting

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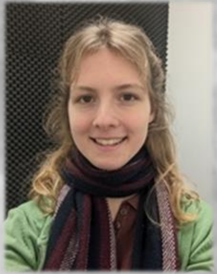
Moes, Vliem *et al.* 2023, *Nano Letters* (under review)

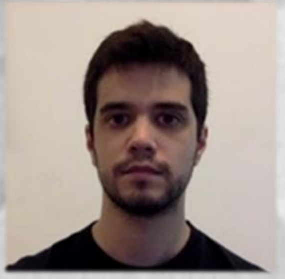
Consortium

Debye Institute for Nanomaterials Science

Jesper Moes



Jara Vliem



Pedro Melo

Thomas Wigmans

Rafael Mendes

Ella van Brenk

Ingmar Swart

Zeila Zanolli

Daniel Vanmaekelbergh

Institute for Theoretical Physics

Lucas Maisel

Sebastiaan Koerhuis

Henk Stoof

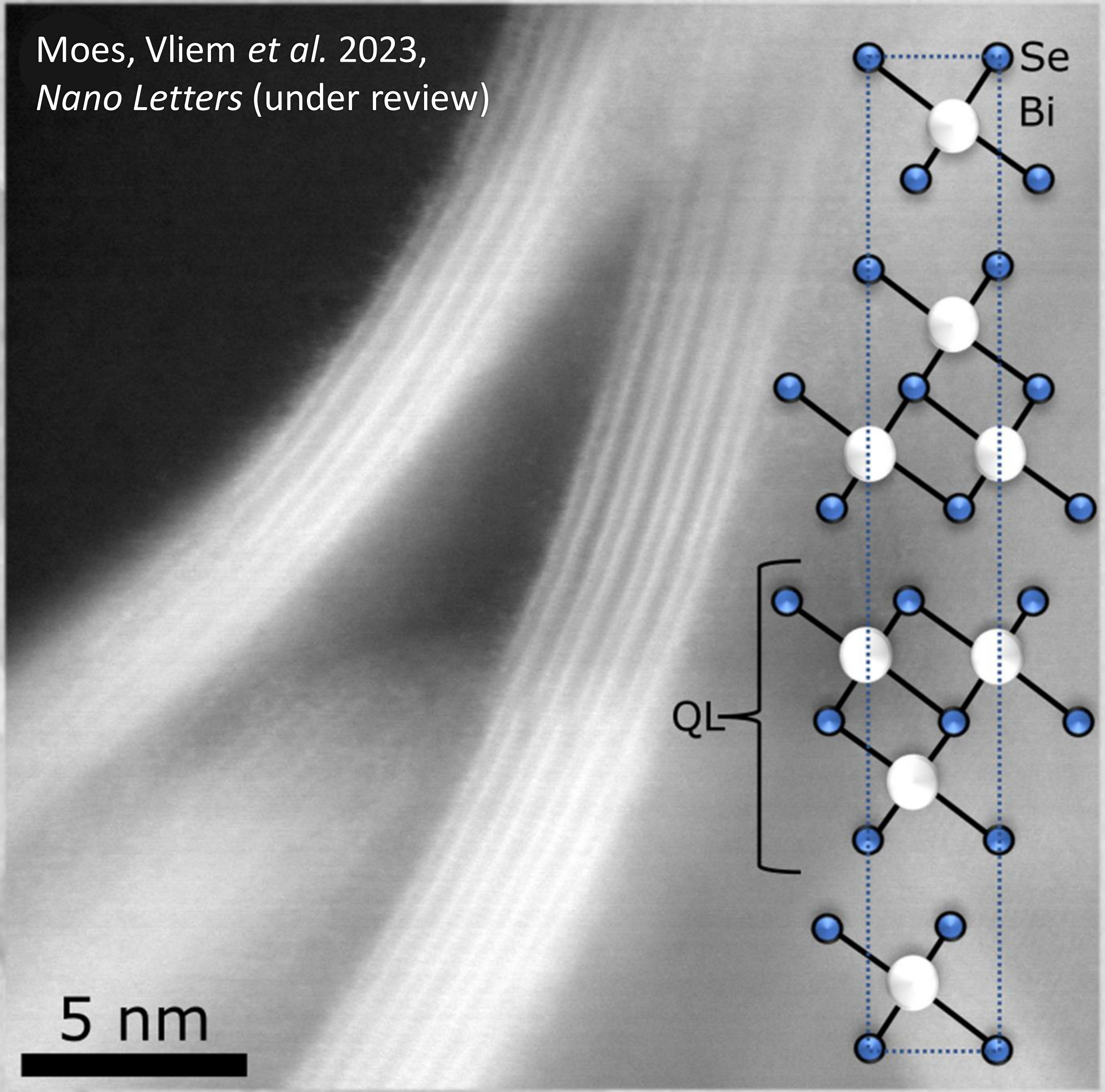
Université de Lille

Institute for Electronics, Microelectronics and Nanotechnology

Christophe Delerue

The Bi_2Se_3 crystal

- Layered structure: quintuple layers (QLs)
- 1 QL: Se–Bi–Se–Bi–Se
- QLs held together by van der Waals forces



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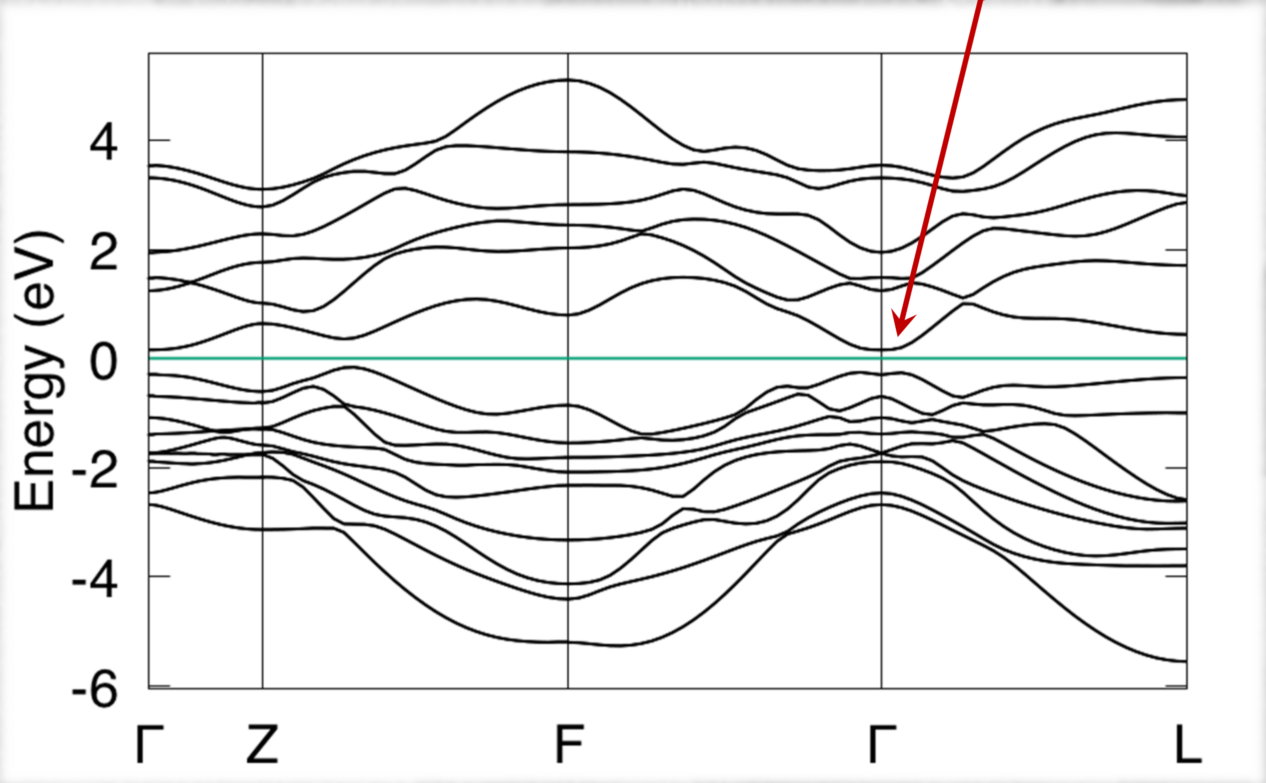
Bi_2Se_3 as a bulk topological insulator

Band inversion
around the Γ point



WannierTools

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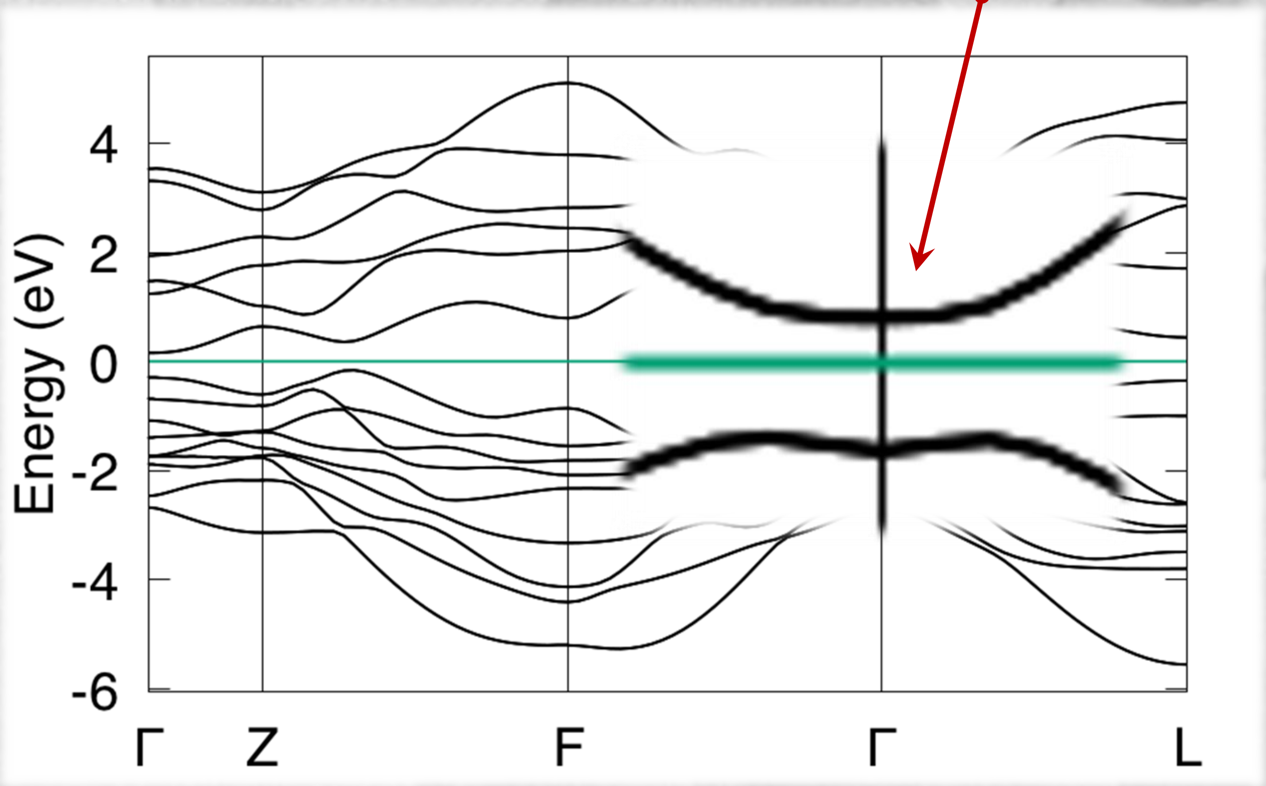

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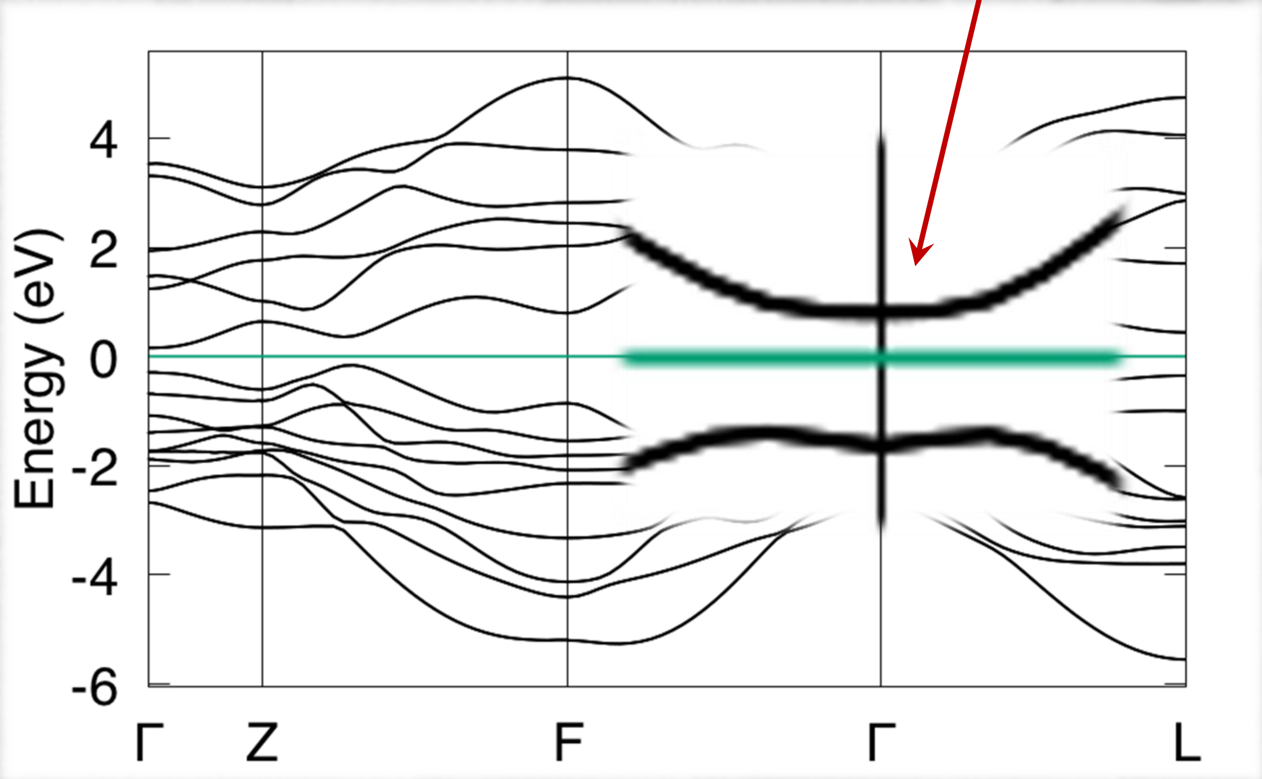
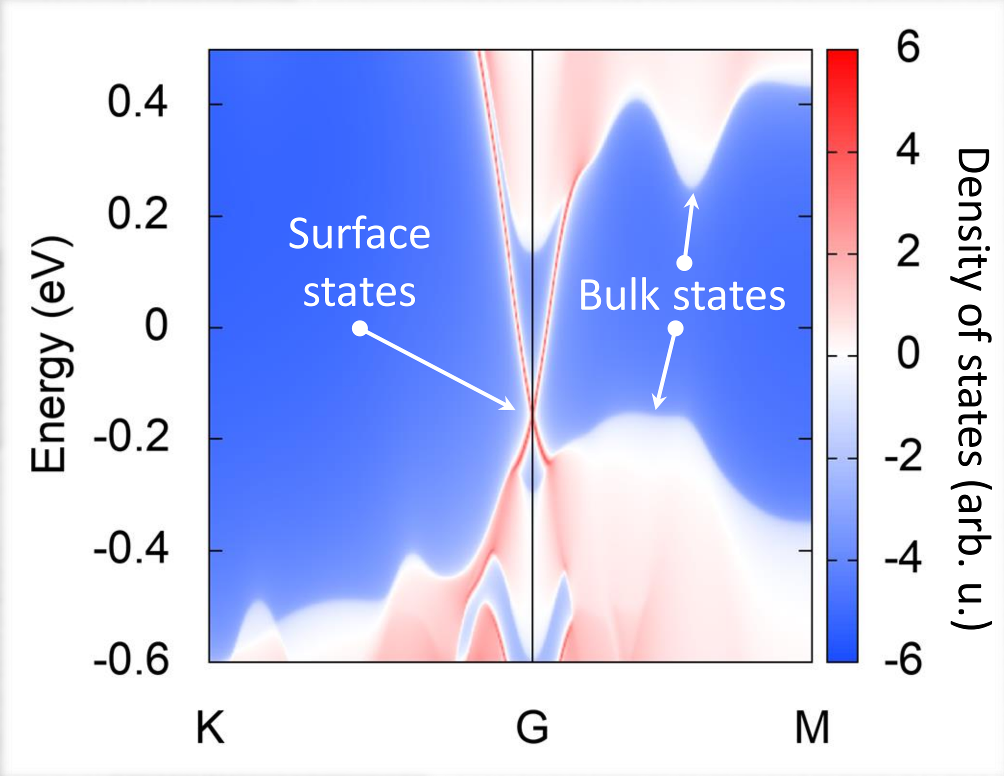
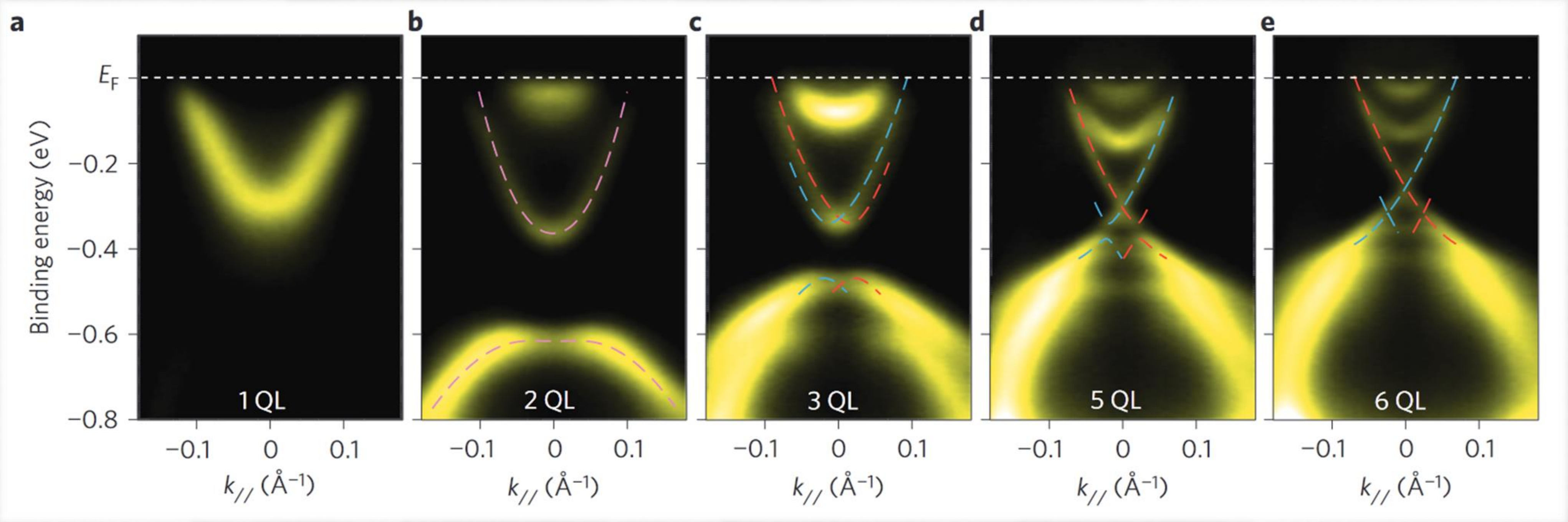




WannierTools

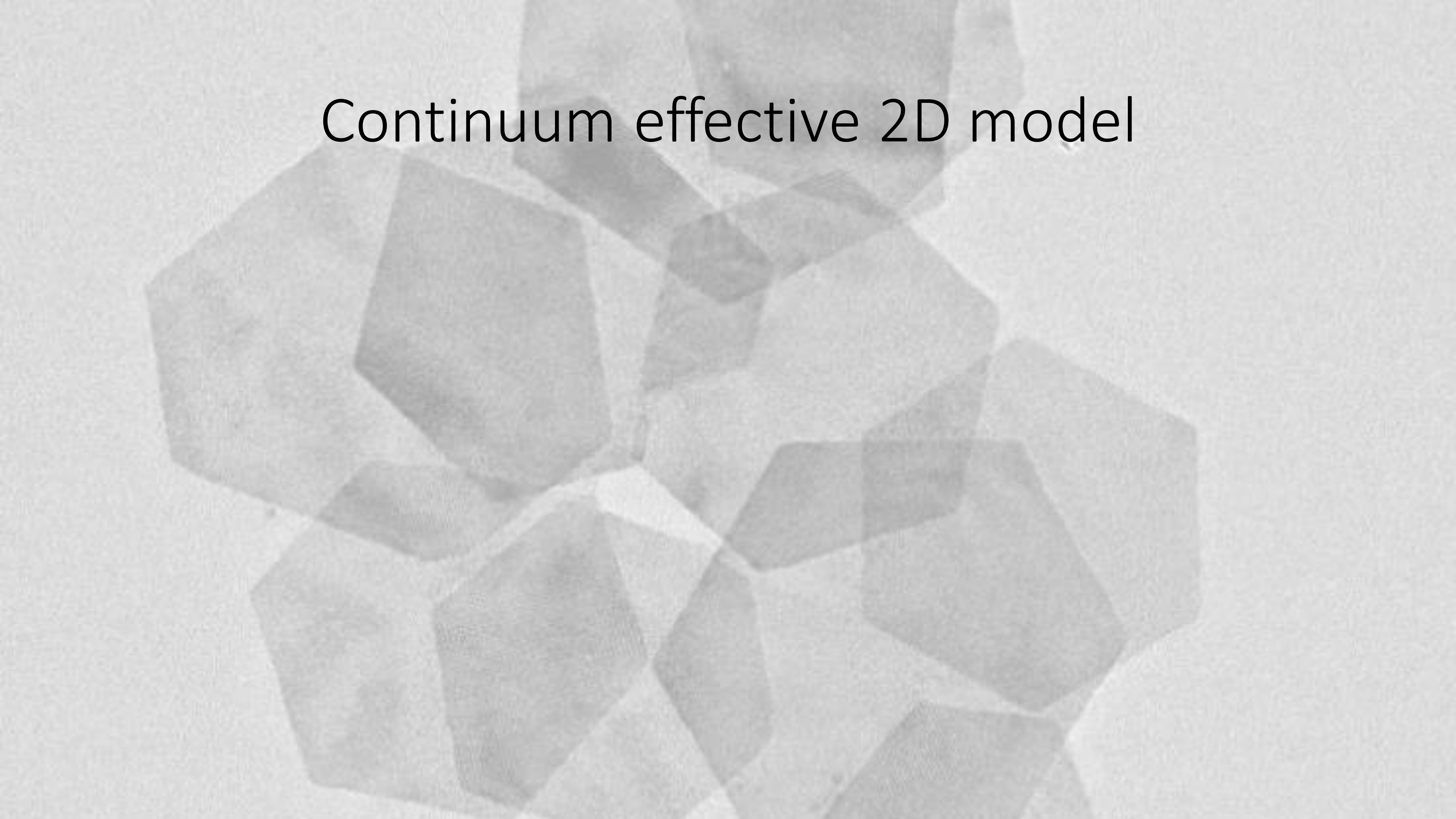
From 3D to 2D

- As the number of QLs decreases, the surface states become gapped
- Crossover to a (possible) quantum spin-Hall phase



Zhang *et al.*, *Nature Physics* 6, 584-588 (2010)

Continuum effective 2D model

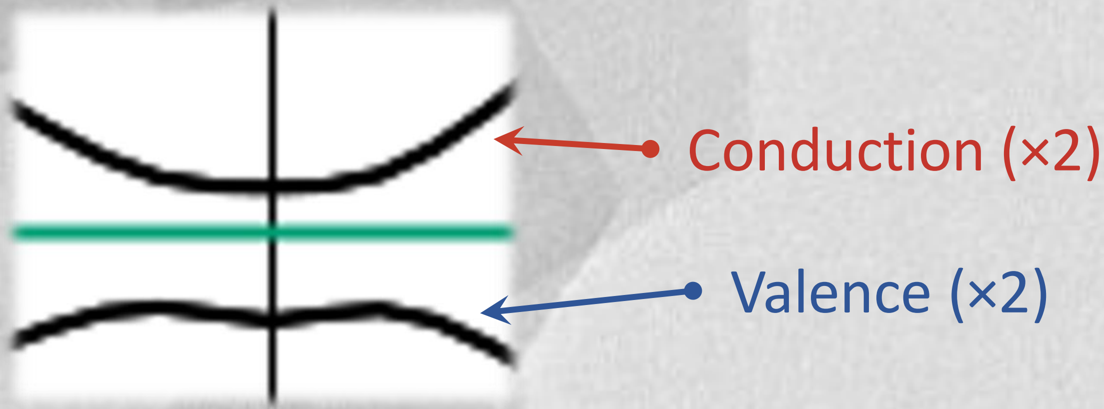


Continuum effective 2D model

1. Start from *the* 3D $\boldsymbol{k} \cdot \boldsymbol{p}$ model around Γ (Zhang et al., 2009)

$$H^{3D}(\boldsymbol{k}) = \epsilon_0(\boldsymbol{k})\mathbb{I}_{4\times4} + \begin{bmatrix} \mathcal{M}(\boldsymbol{k}) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}(\boldsymbol{k}) & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}(\boldsymbol{k}) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}(\boldsymbol{k}) \end{bmatrix}$$

$$\epsilon_0(\boldsymbol{k}) = C + D_1 k_z^2 + D_2\left(k_x^2 + k_y^2\right)$$
$$\mathcal{M}(\boldsymbol{k}) = M - B_1 k_z^2 - B_2\left(k_x^2 + k_y^2\right)$$



Continuum effective 2D model

1. Start from *the* 3D $\boldsymbol{k} \cdot \boldsymbol{p}$ model around Γ (Zhang et al., 2009)

2. Solve it in a slab geometry (finite L_z) for $k_x = k_y = 0$

$$H^{3\mathrm{D}}(0, 0, -i\partial_z)\Psi_n(z) = E_n\Psi_n(z), \quad \Psi_n(\pm L_z/2) = 0$$

Continuum effective 2D model

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2. Solve it in a slab geometry (finite L_z) for $k_x = k_y = 0$

3. Obtain an **effective 2D model** by projecting on the full Hamiltonian

$$H_{nm}^{\mathrm{2D}}(k_x, k_y) = \langle \Psi_n | H^{\mathrm{3D}}(k_x, k_y, -i\partial_z) | \Psi_m \rangle$$

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Key point: restrict to a **finite subspace**!

“Traditional” 4-band model

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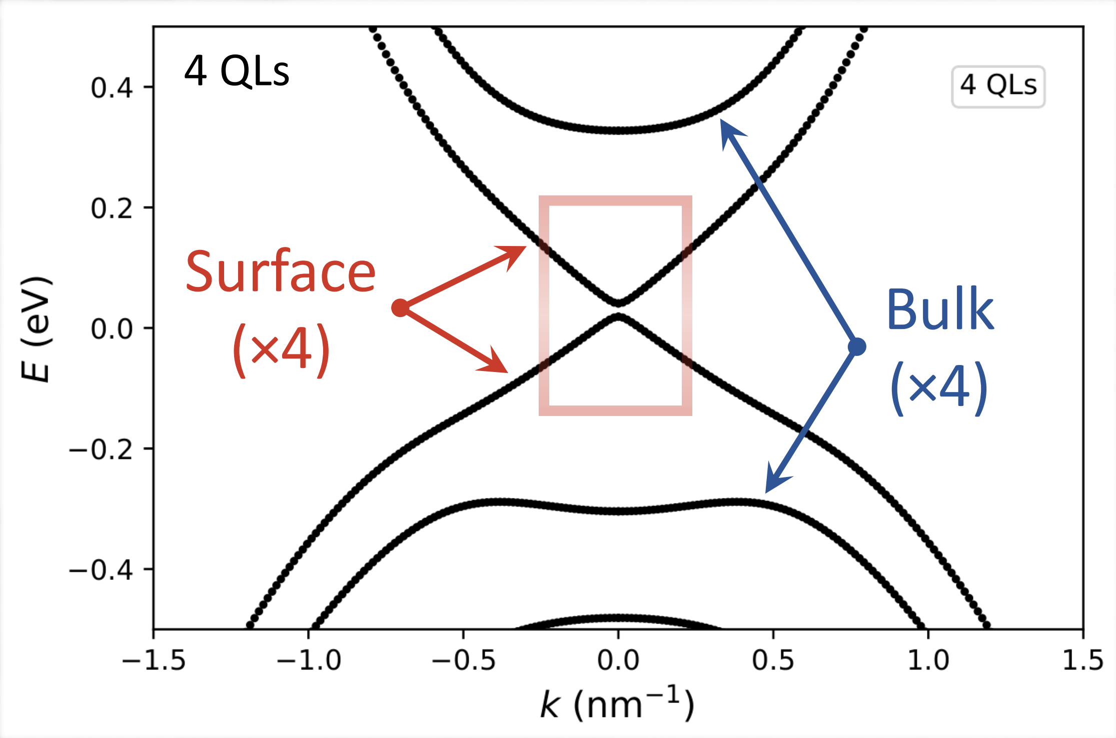
- Describes only the surface states



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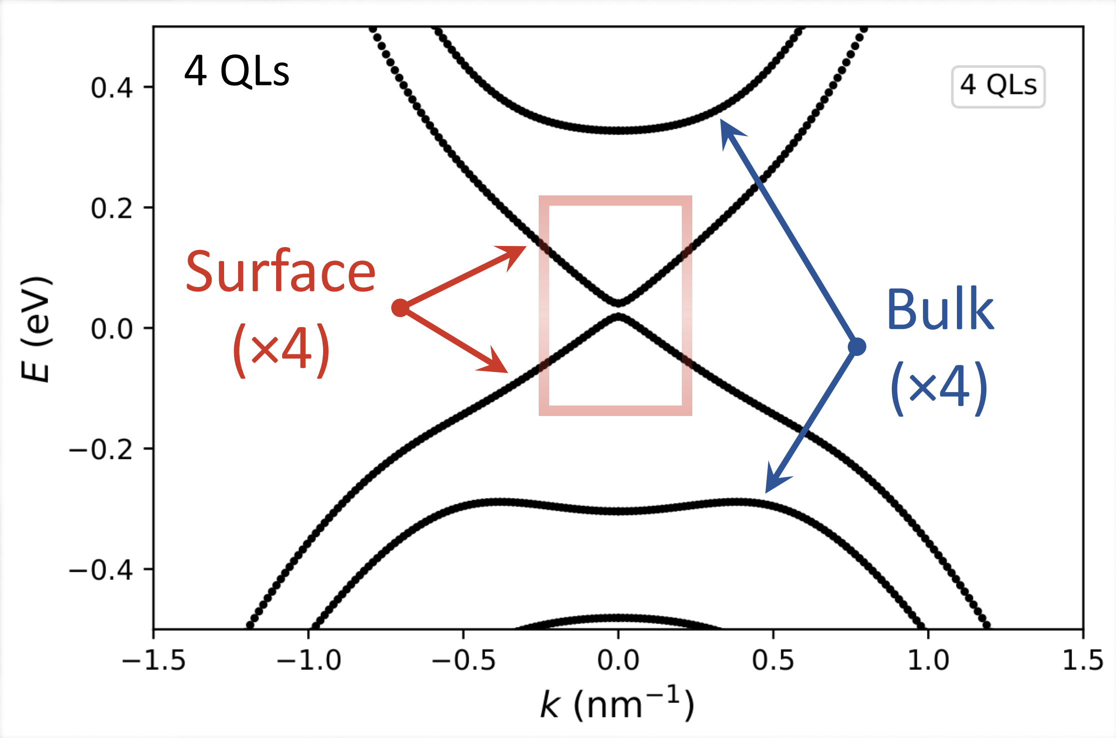

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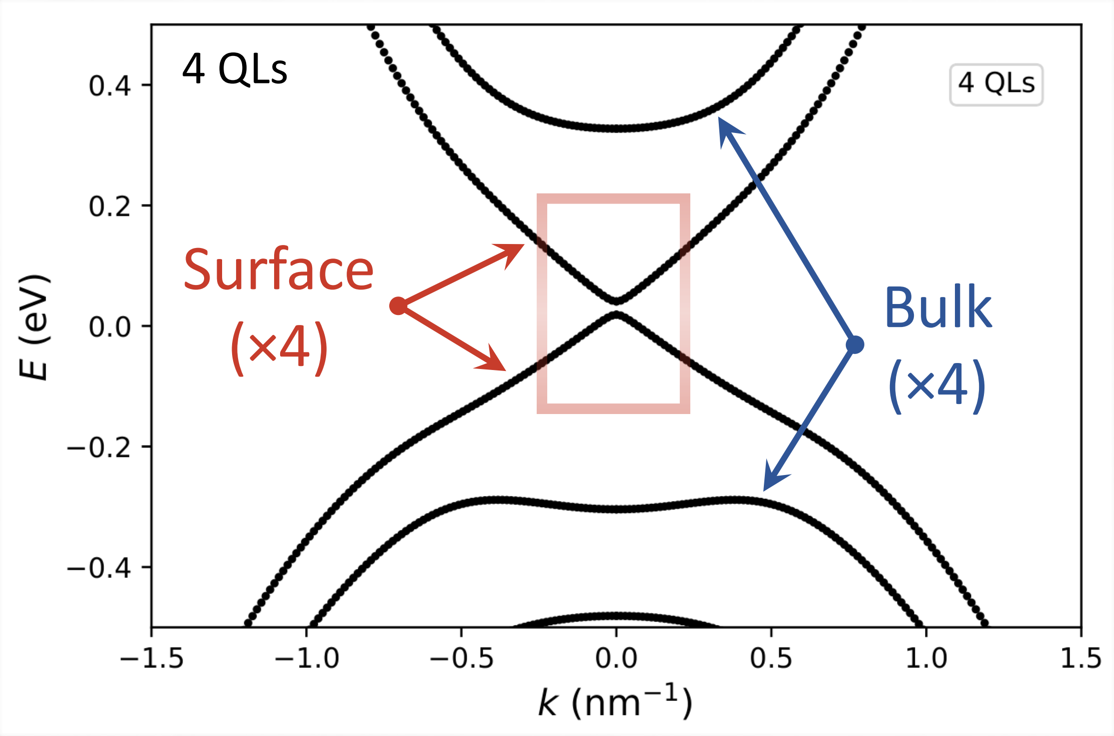
Number of QLs	$k \cdot p$ theory	Experiments, DFT
1	Trivial	Trivial
2	Trivial	Trivial
3	QSH	QSH
4	Trivial	QSH
5	Trivial	QSH
6	QSH	(Unclear)



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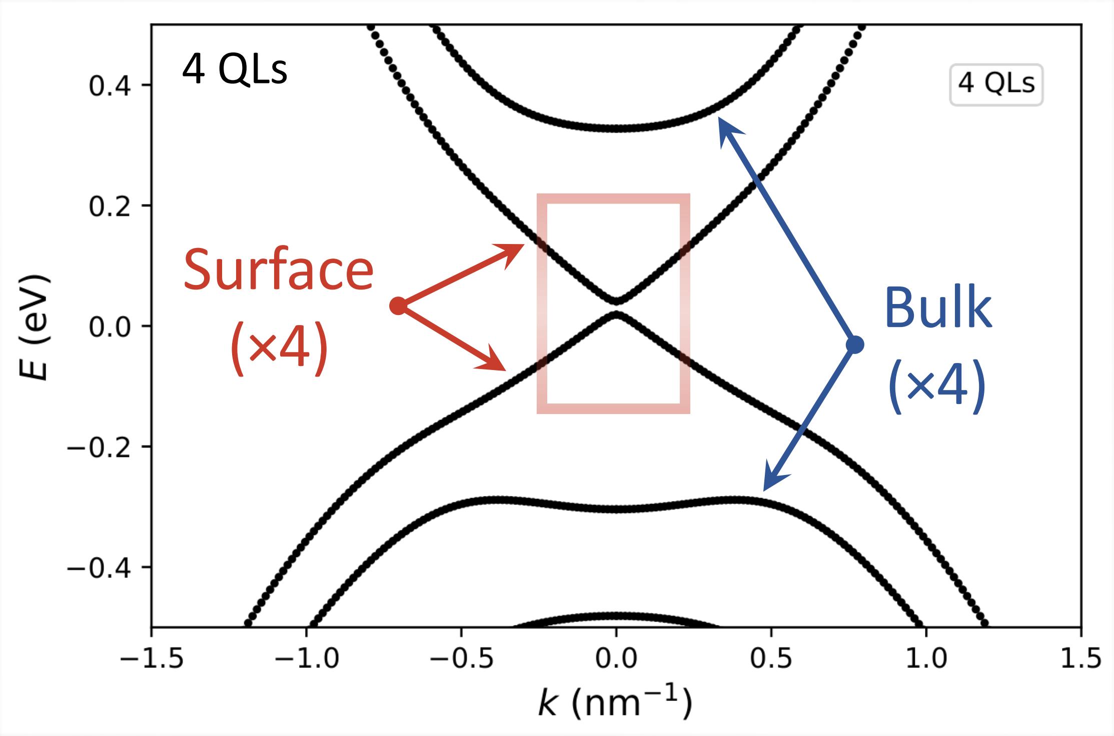
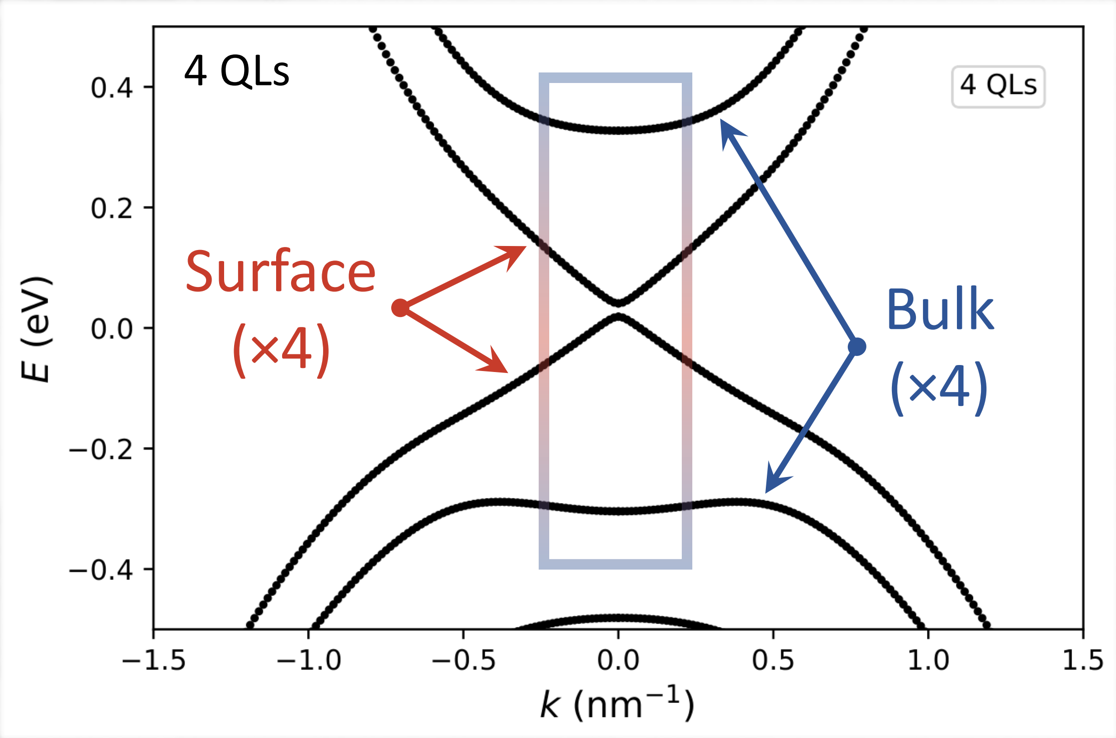


→ Can we do better?

New 8-band model

New 8-band model

- Describes the surface states and the first set of bulk states together



New 8-band model

- Describes the surface states and the first set of bulk states together
- Topology **agrees** with experiments and DFT!

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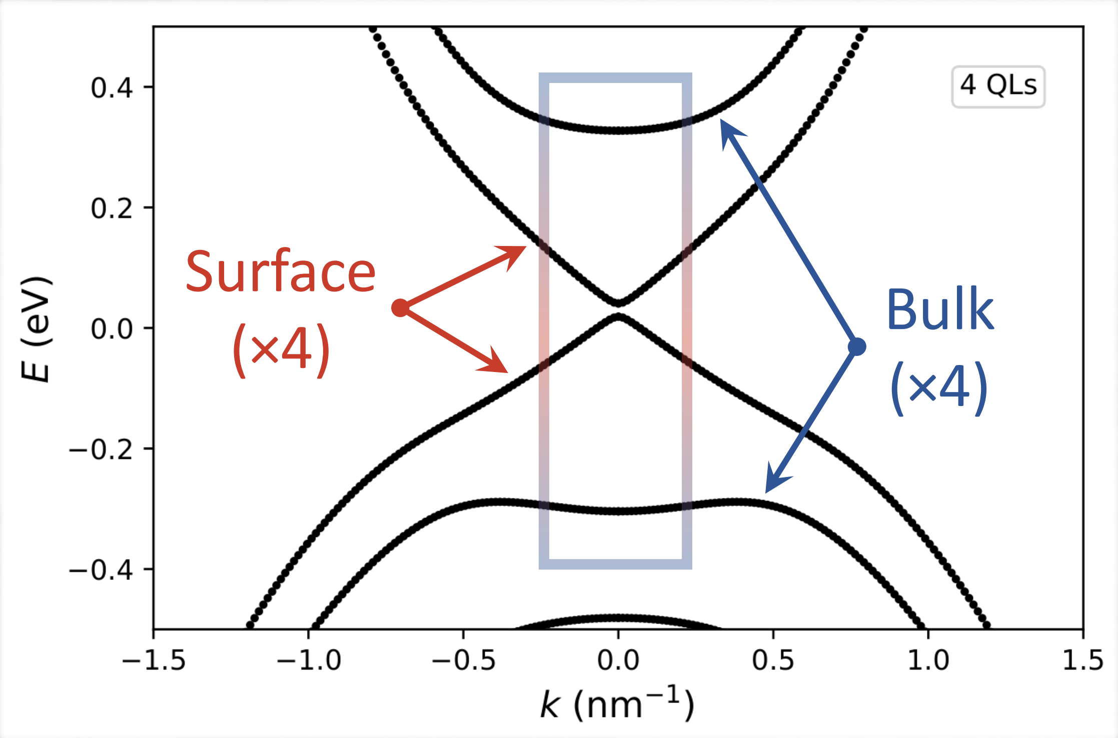
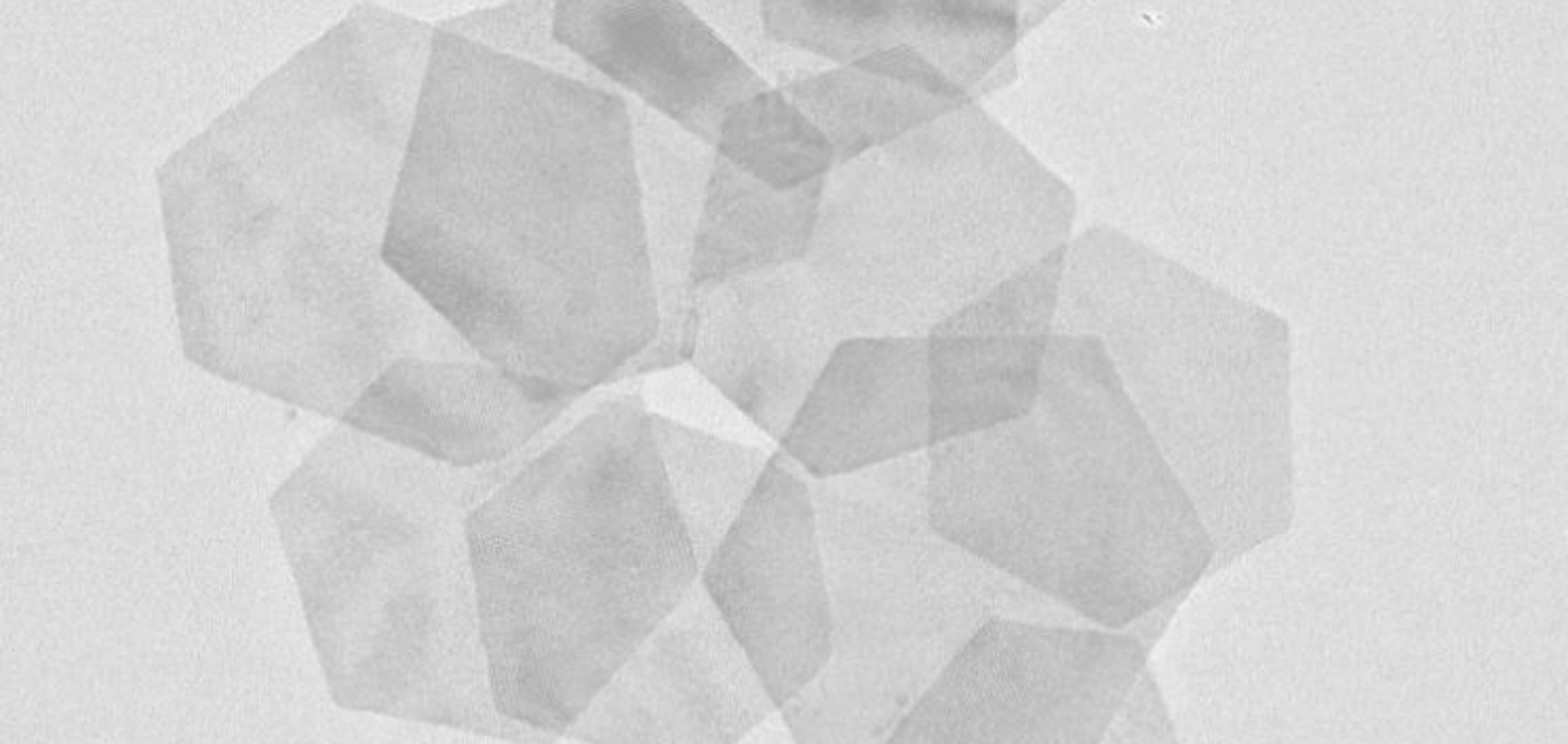
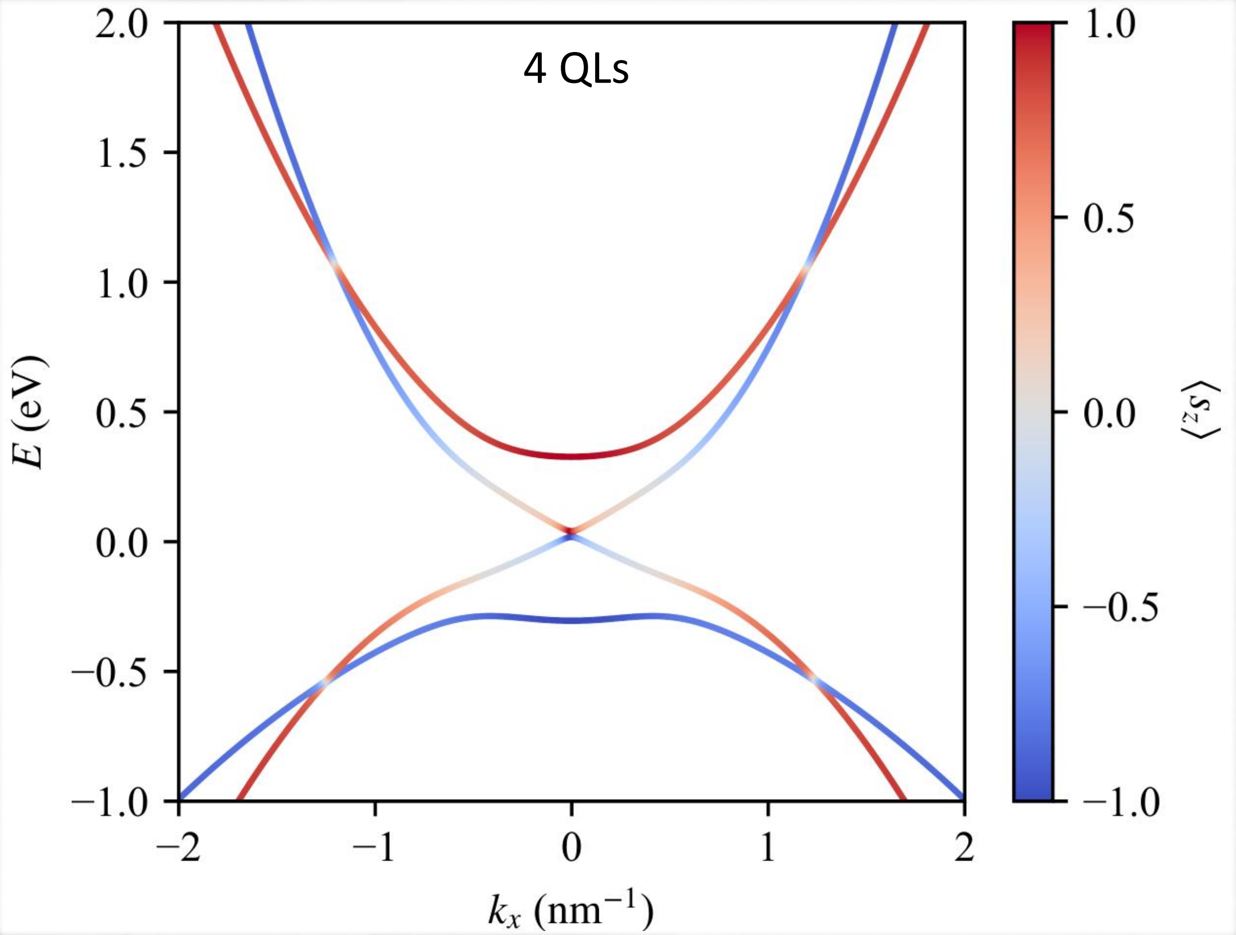


Topology in the 8-band model



Topology in the 8-band model

- Can be understood by tracking the direction of the **spin** as a function of the momentum



Maisel Licerán *et al.*, arXiv:2309.02792 (2023)

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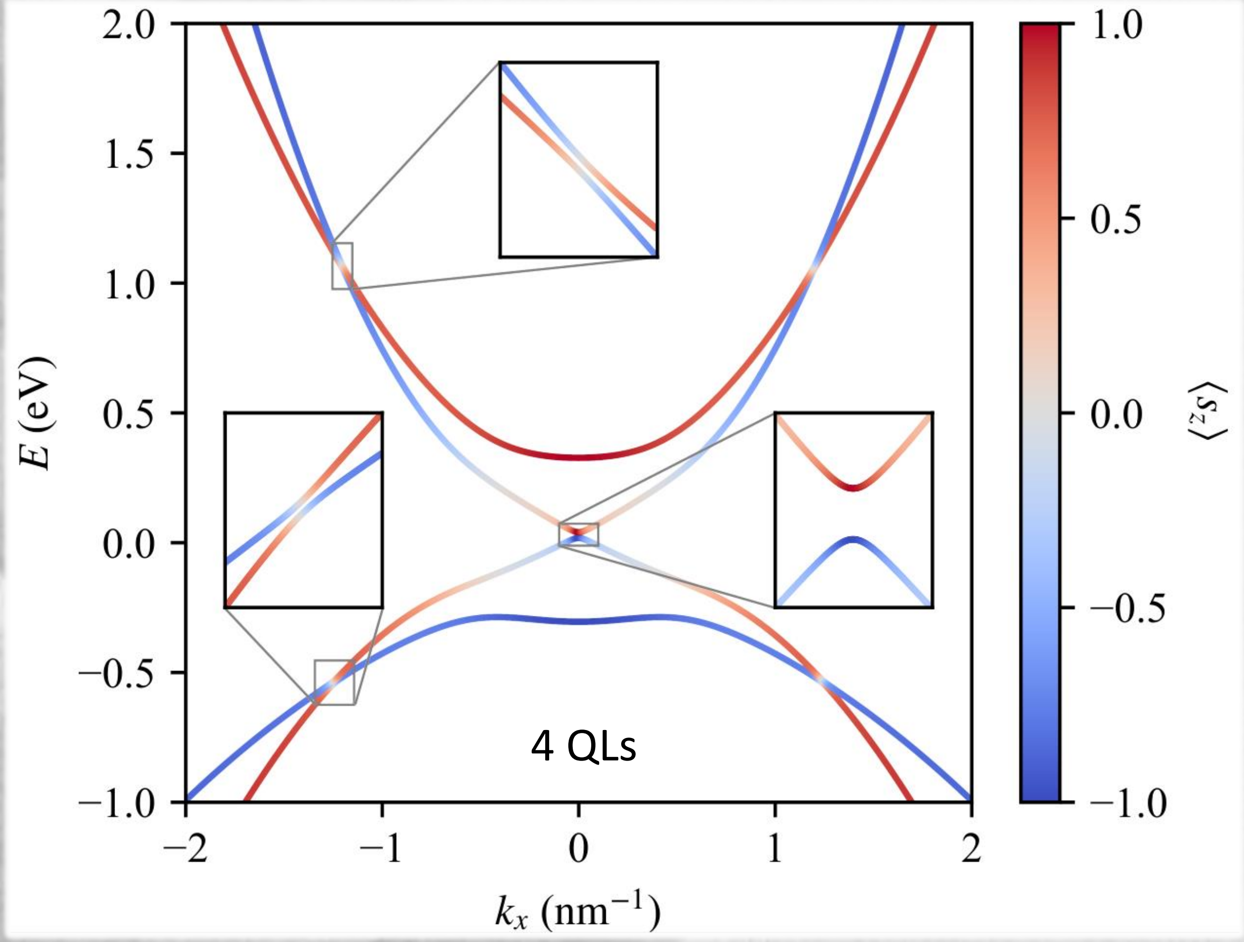
- Can be understood by tracking the direction of the spin as a function of the momentum
- Arises from an **interplay** between surface and bulk



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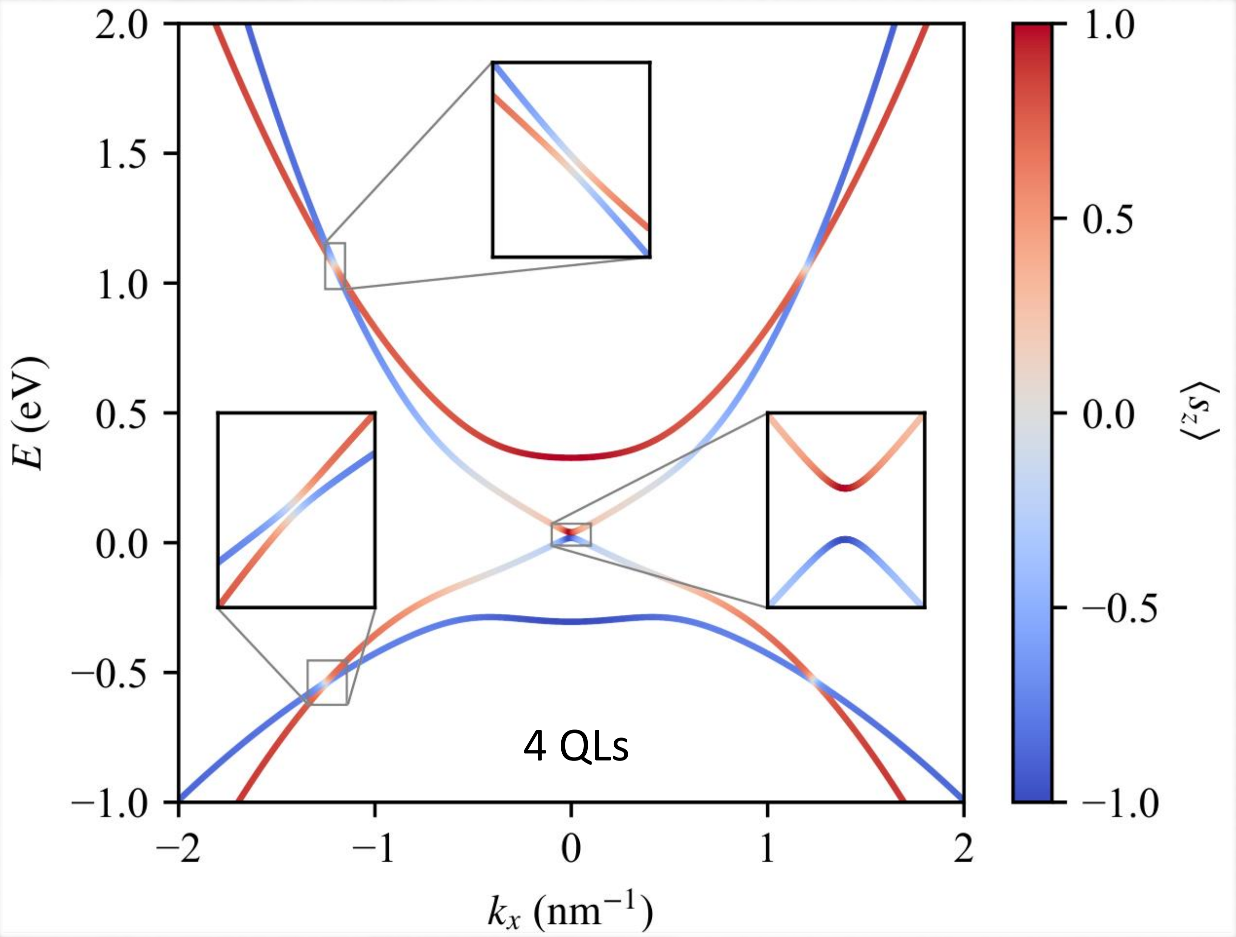

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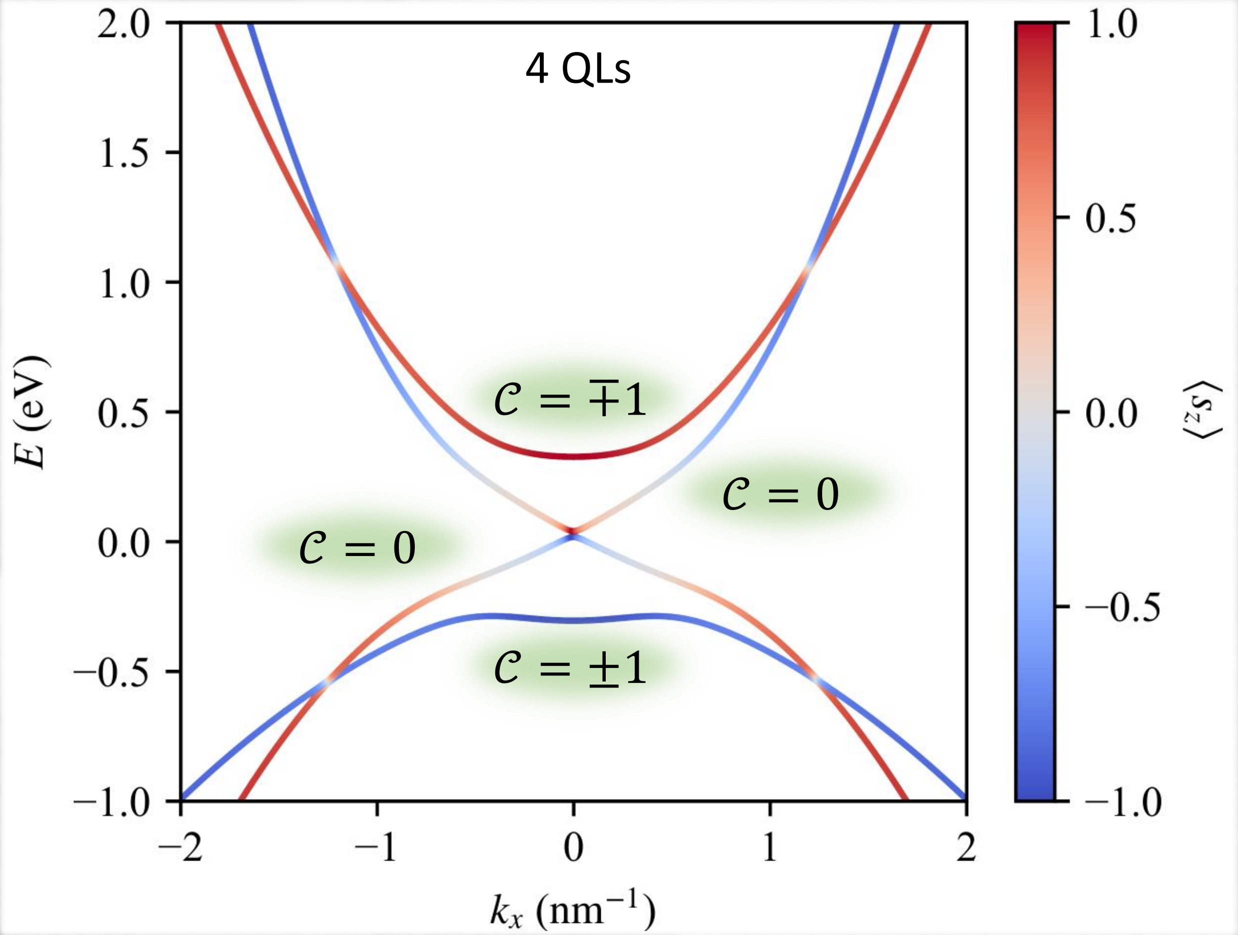
Topology in the 8-band model

- Can be understood by tracking the direction of the spin as a function of the momentum
- Arises from an interplay between surface and bulk
- Band inversion around the Γ point, but also at the avoided crossings
- Surface bands are **trivial**, bulk bands are **topological**



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Edge states comparison (4 QLs)

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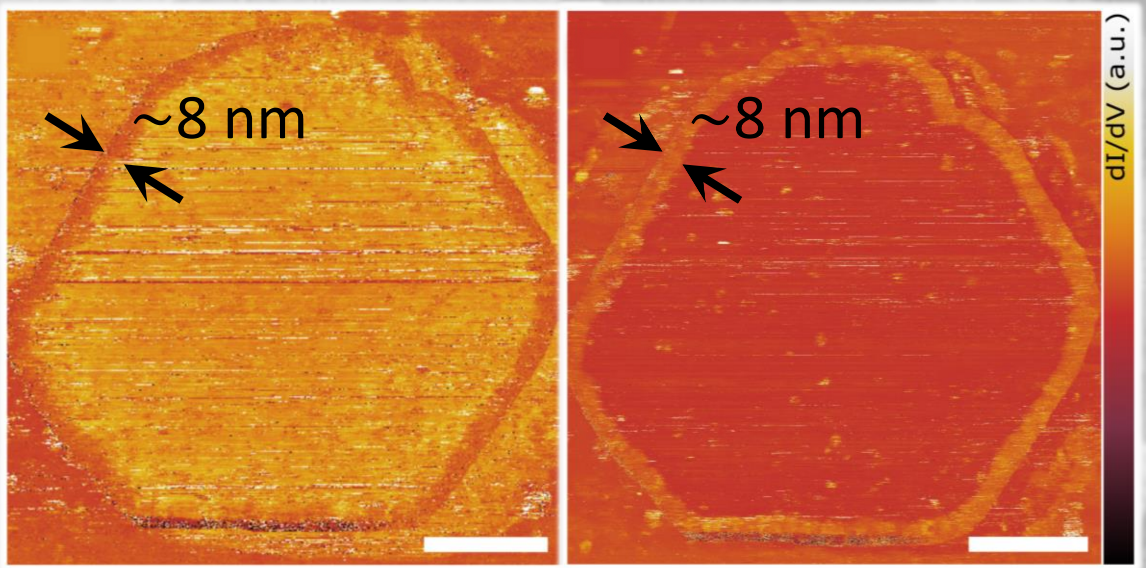

Moes, Vliem *et al.* 2023,
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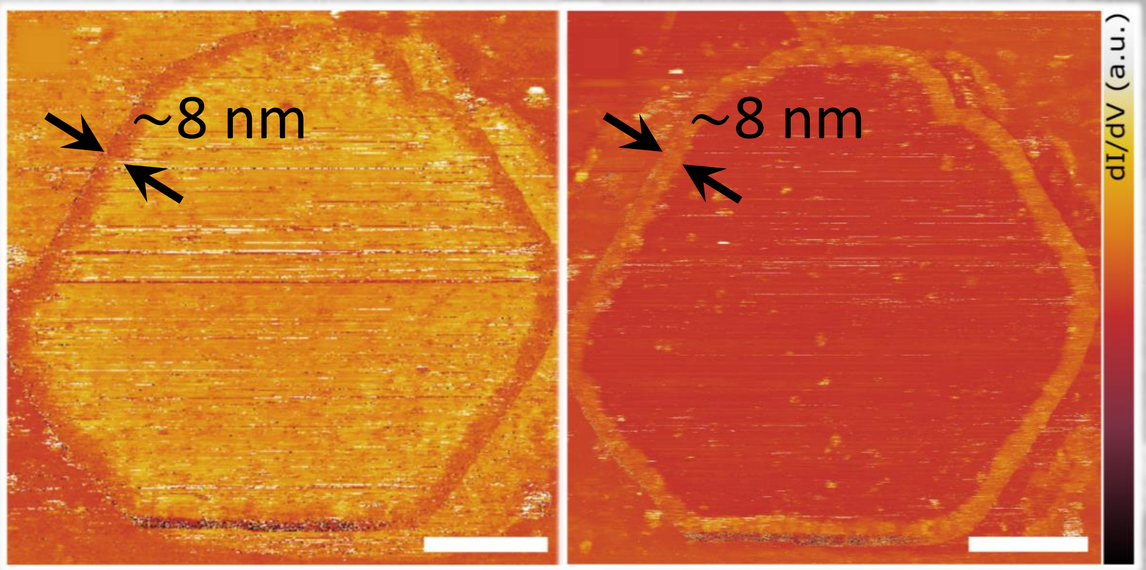

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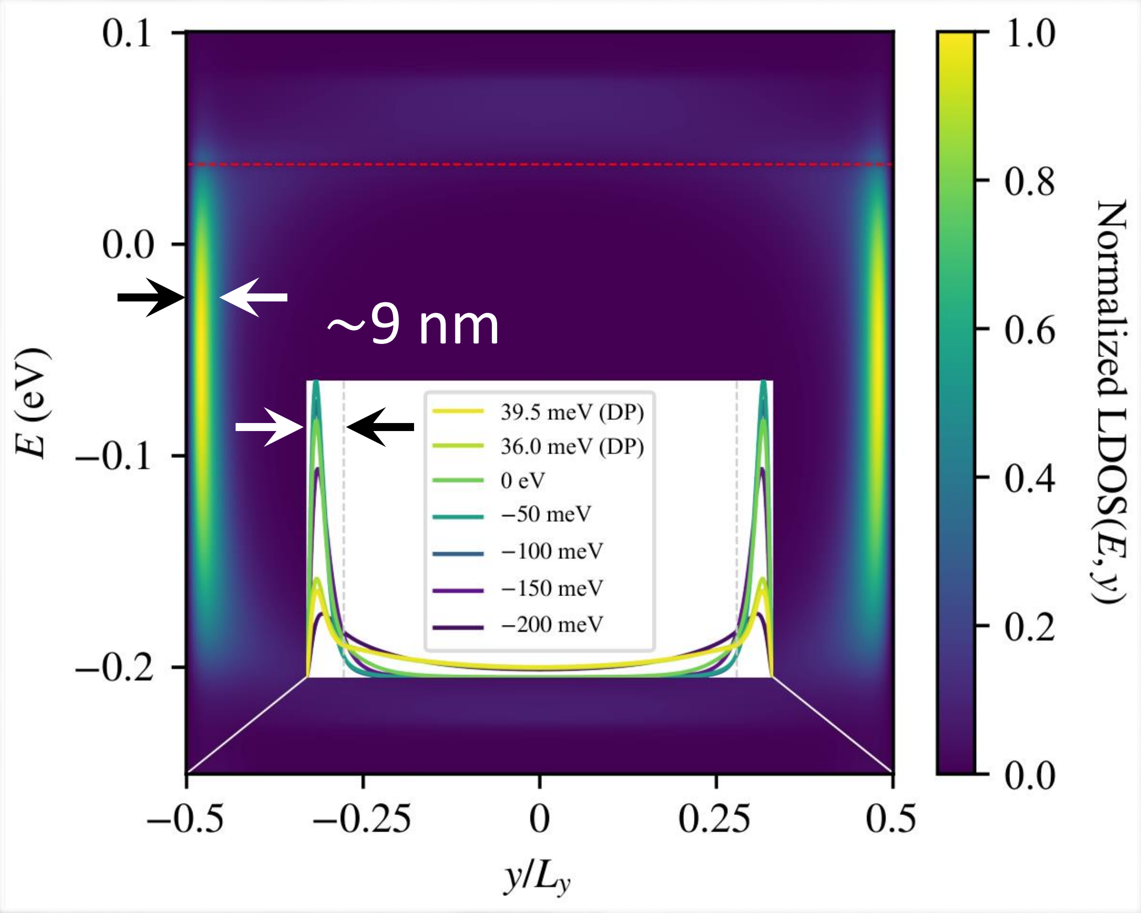

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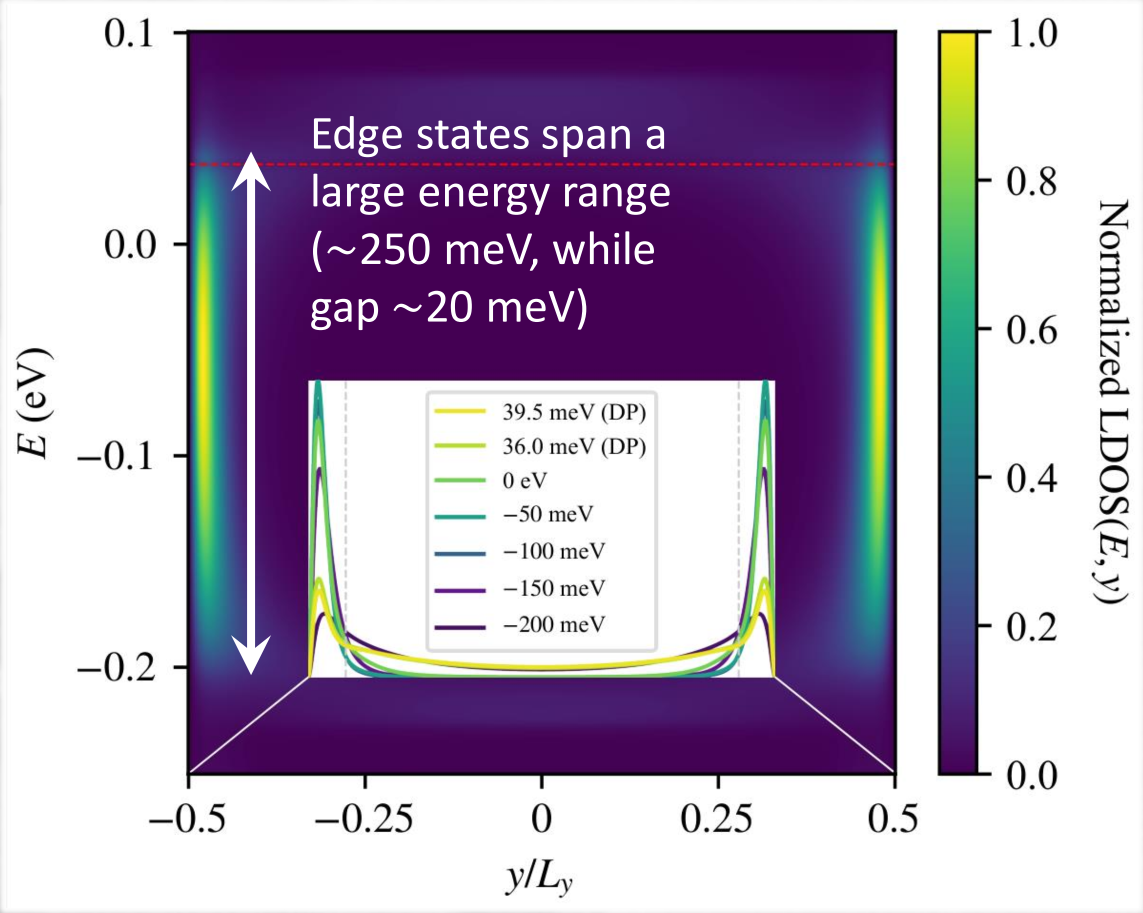

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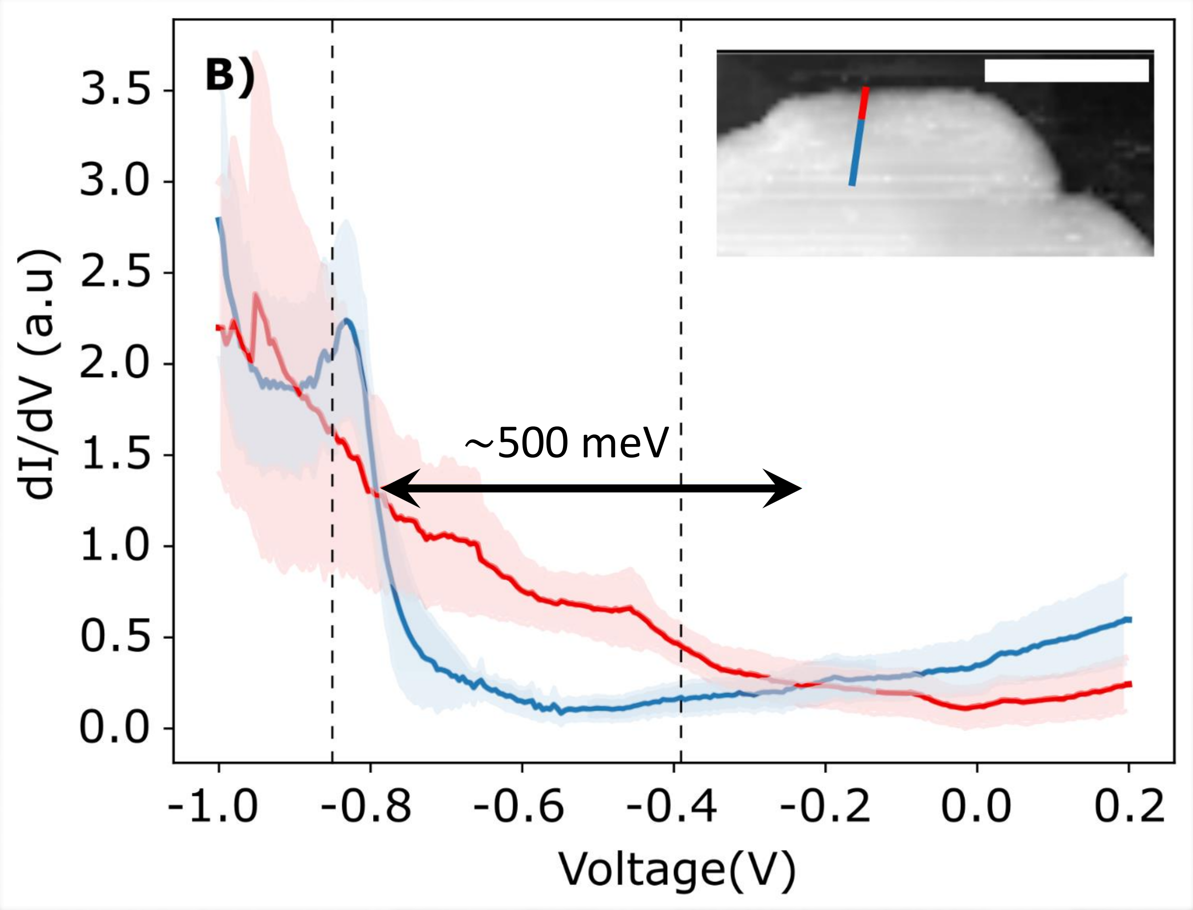

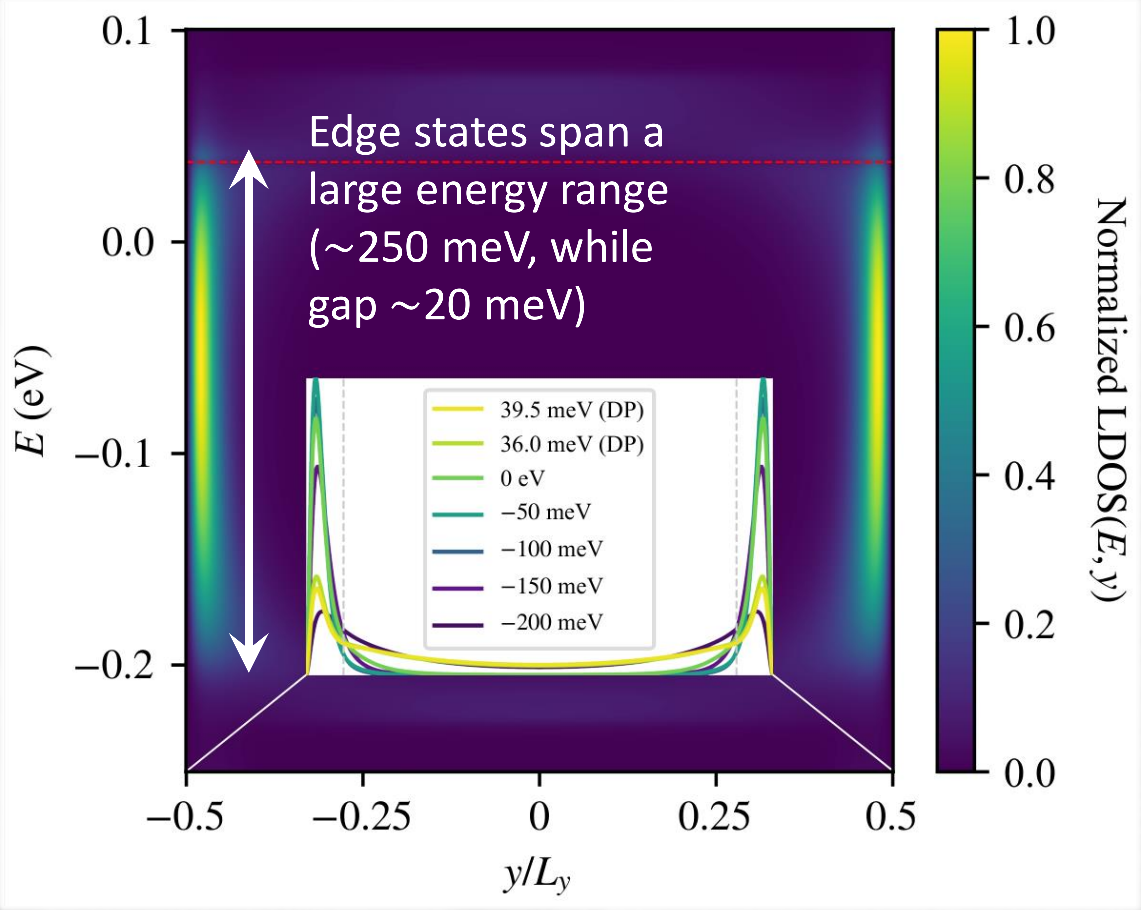

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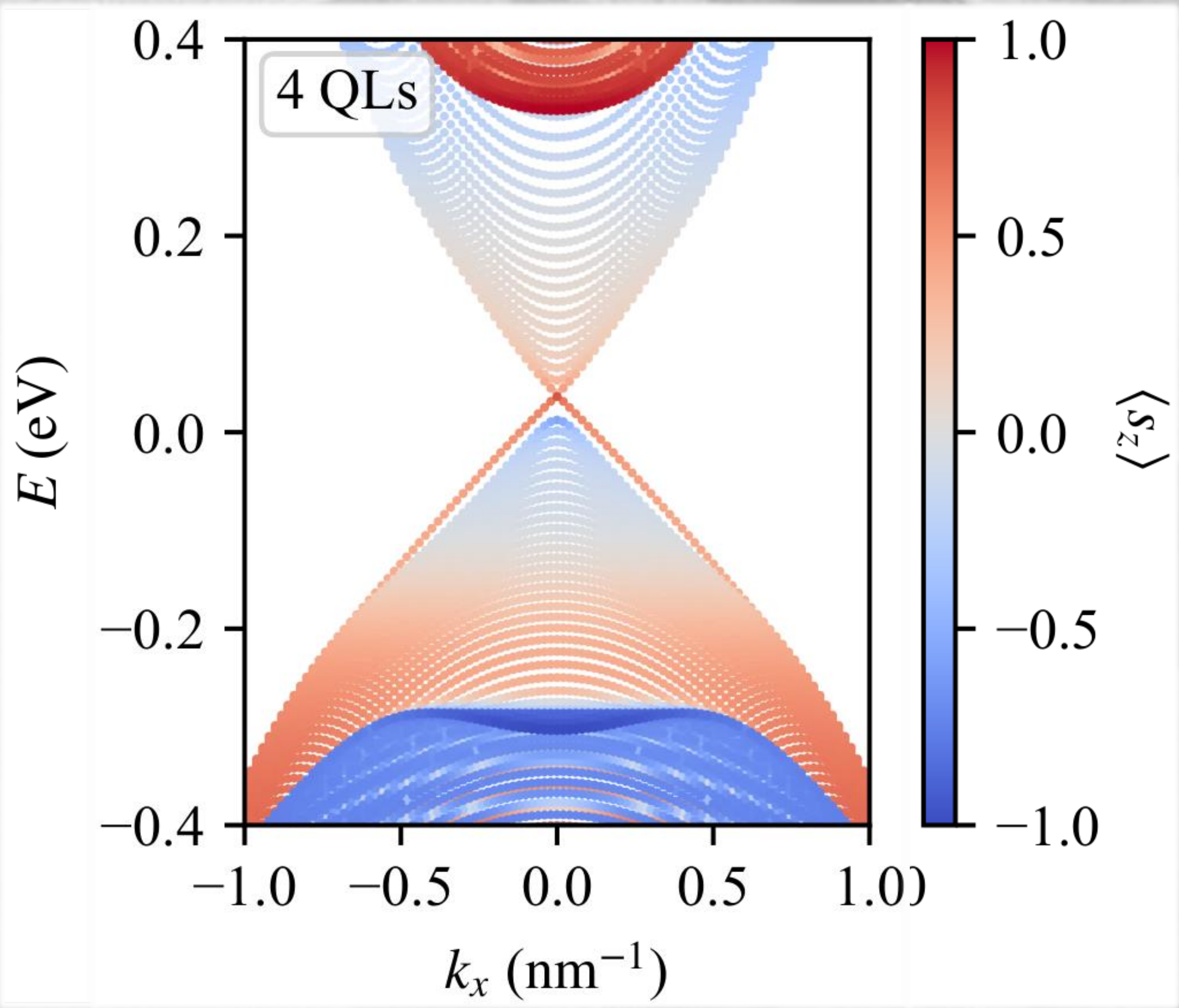

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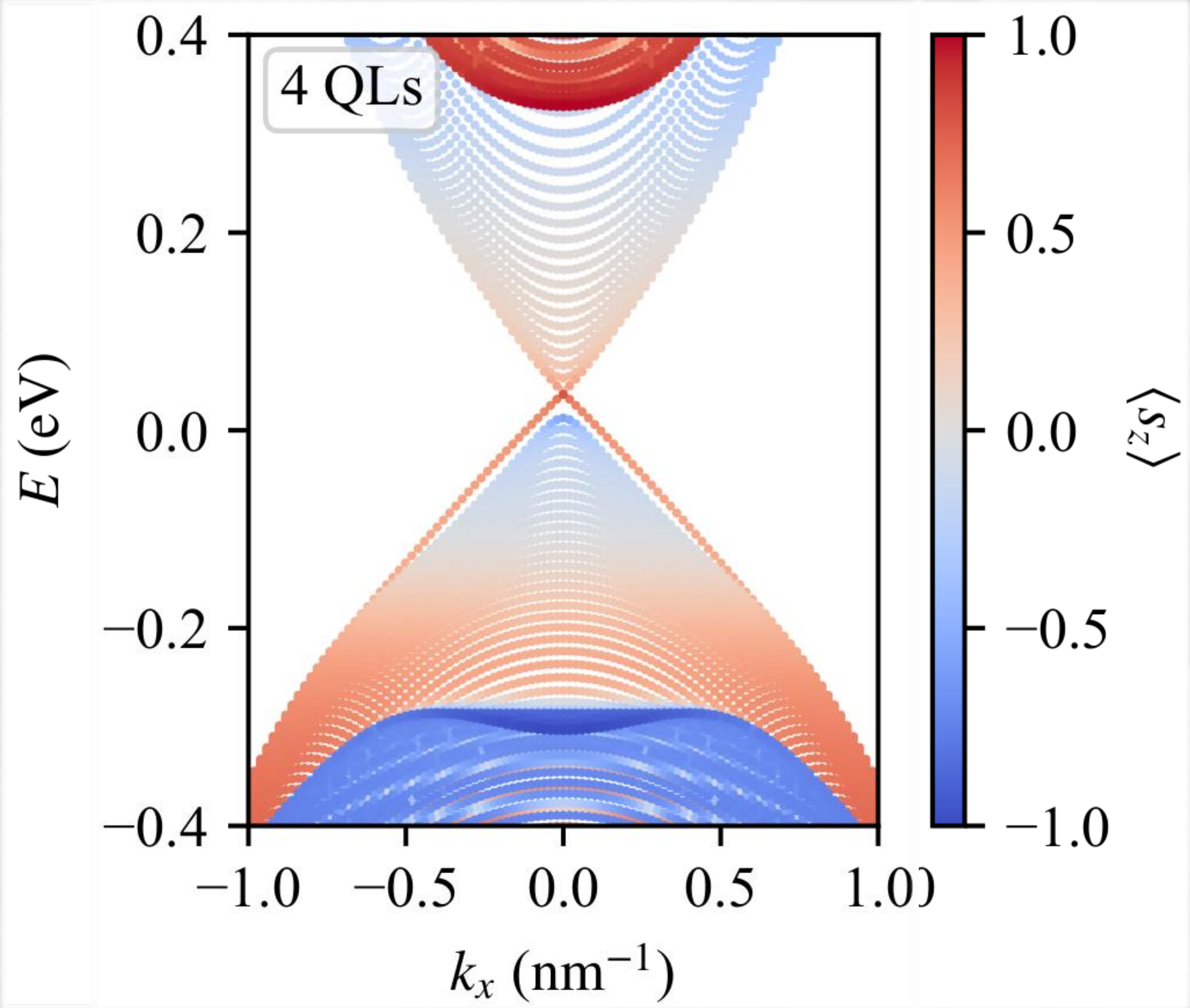

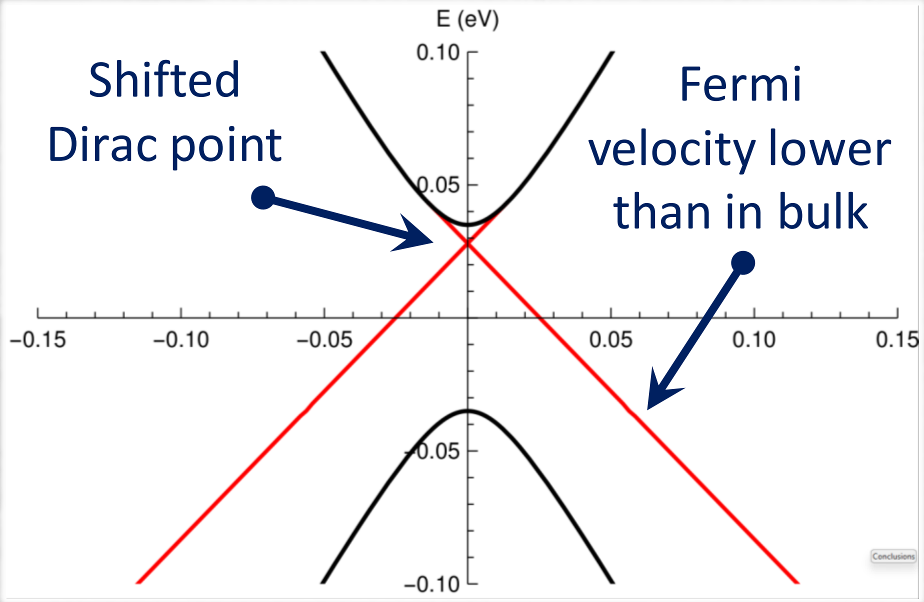

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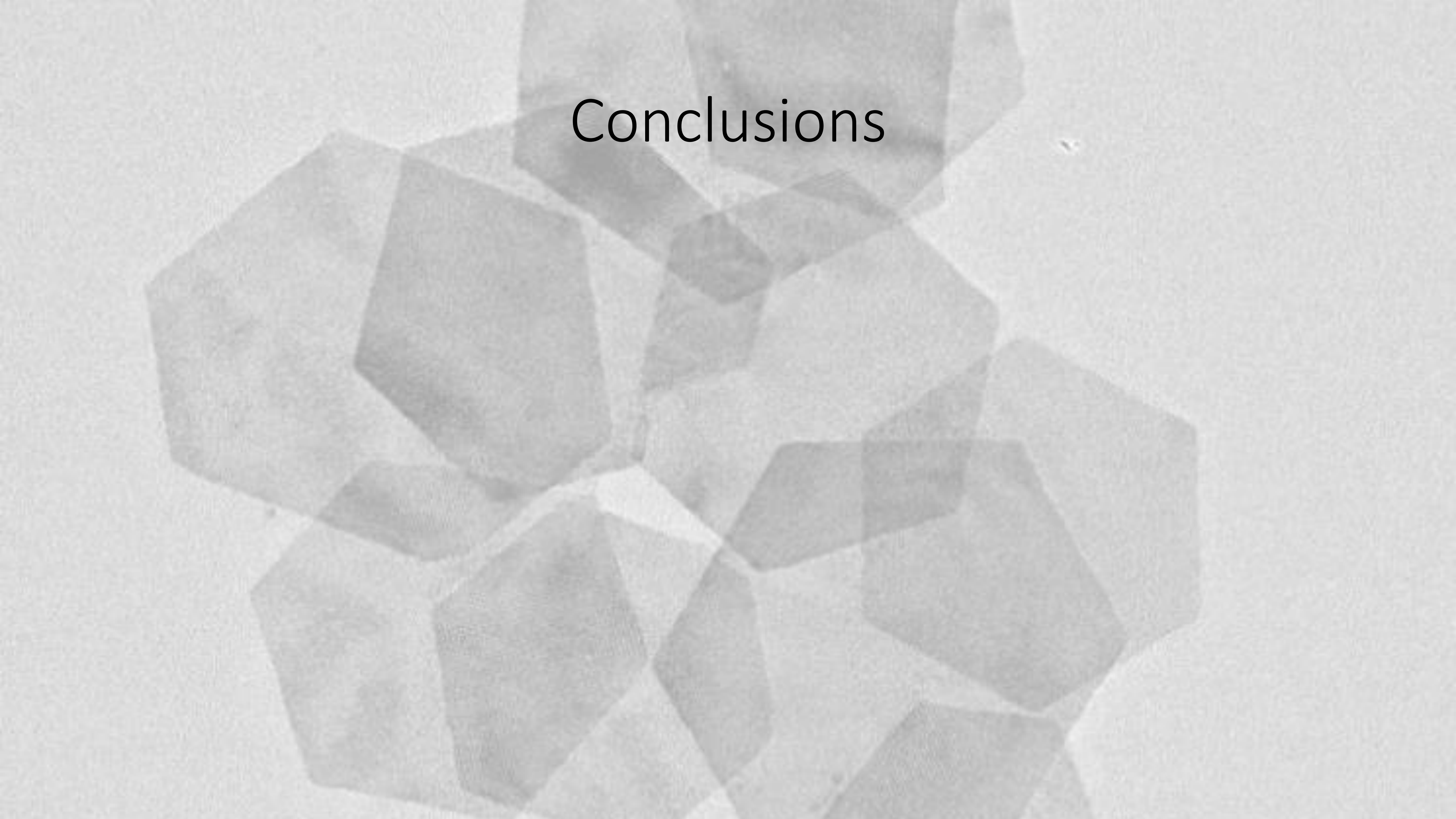
Conclusions



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- Large energy range possibly due to **shifting of the Dirac point** in combination with a **change in Fermi velocity**

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